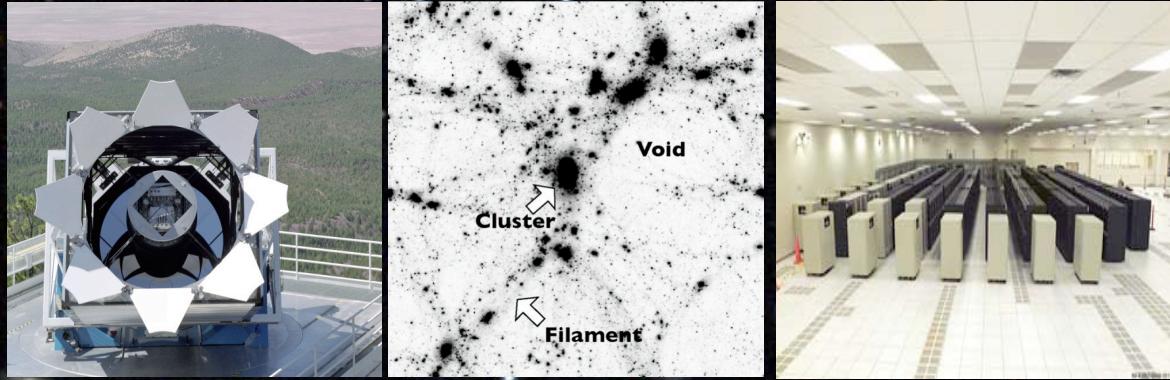
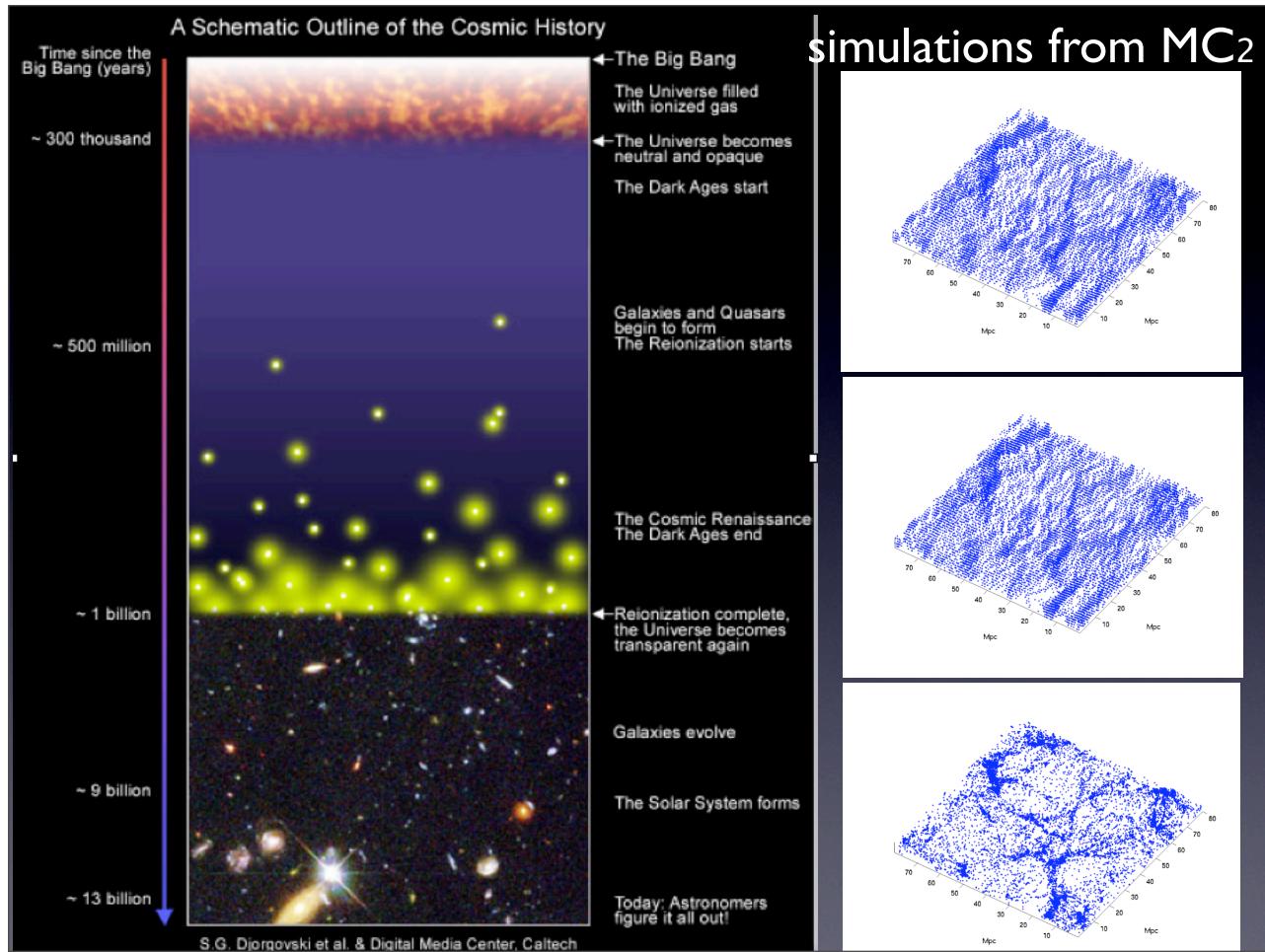


# Cosmic Calibration

Salman Habib, Katrin Heitmann, Dave Higdon, Charlie Nakleleh, and Brian Williams--Los Alamos National Laboratory



Background: A small section of the first light image obtained by the Sloan Digital Sky Survey



# Data Sources

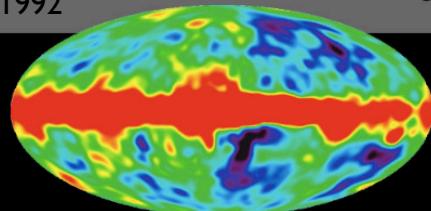
## Cosmic Microwave Background

1965

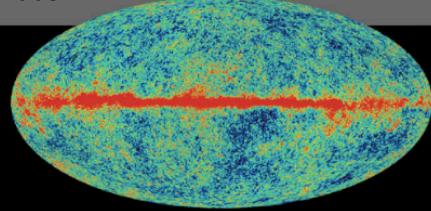
Penzias and Wilson



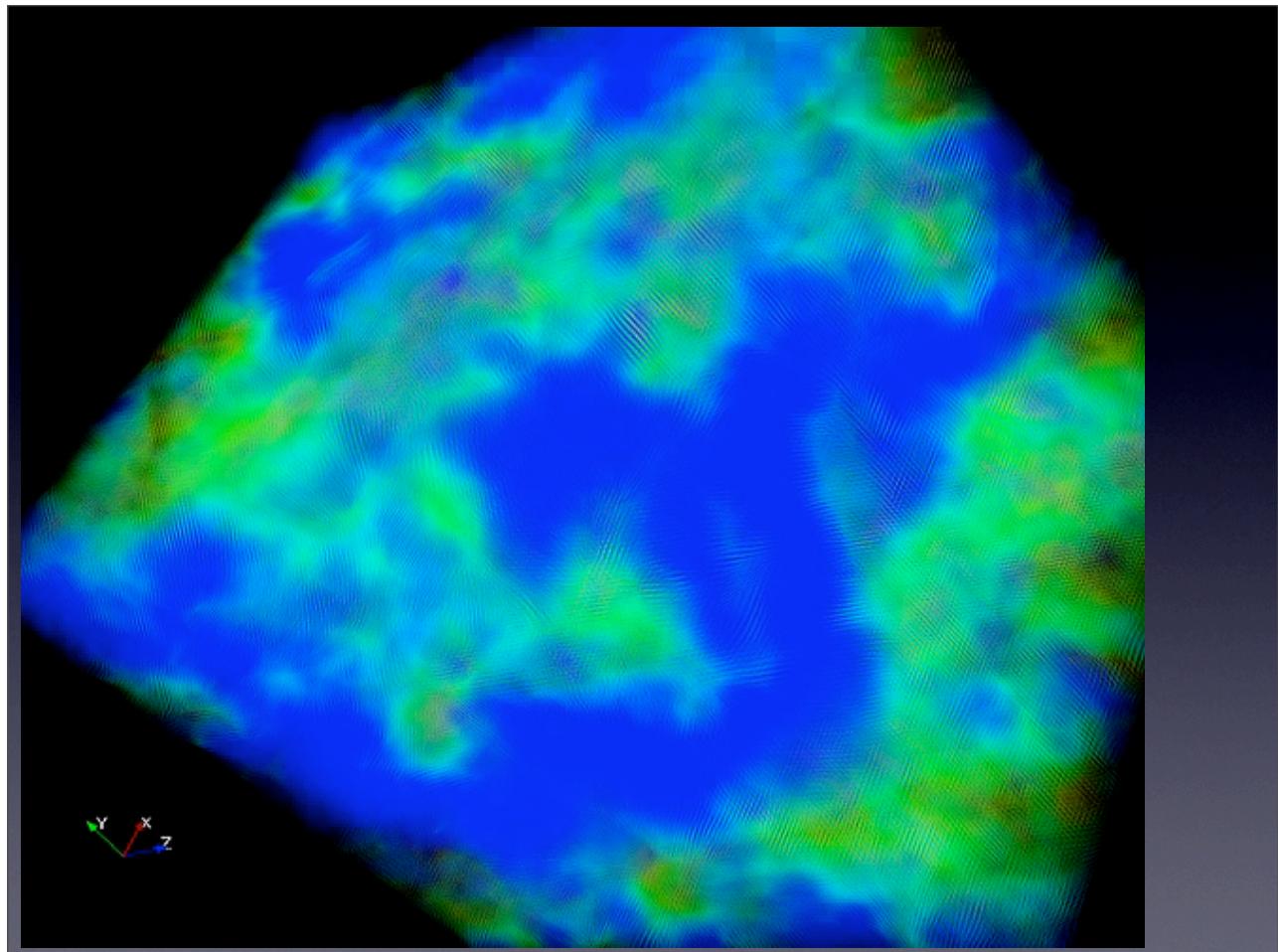
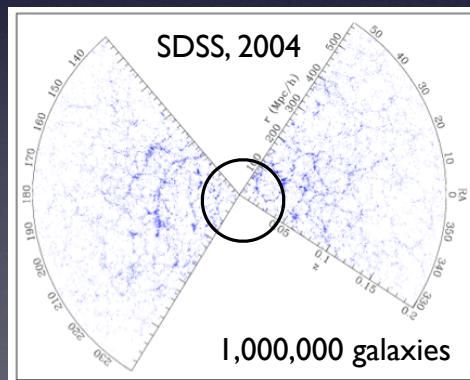
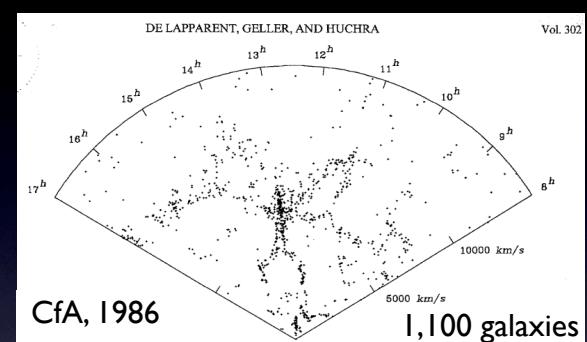
1992



2003

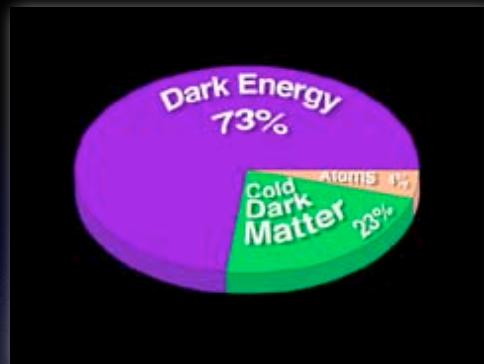


## Large Scale Structure



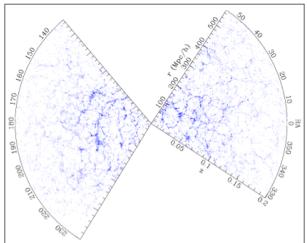
# The Content of the Universe

- “Standard Model of Cosmology”
- ~73% of a mysterious dark energy
- ~23% of an unknown dark matter component
- ~4% of baryons
- constraints on ~20 cosmological parameters, including optical depth, spectral index, hubble constant, ....
- values are known to an accuracy of +/-10%
- for comparison: the parameters of the “Standard Model of Particle Physics” is known with per 0.1% accuracy!

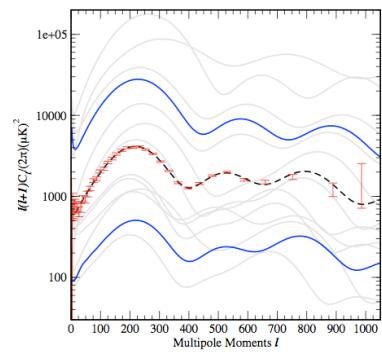
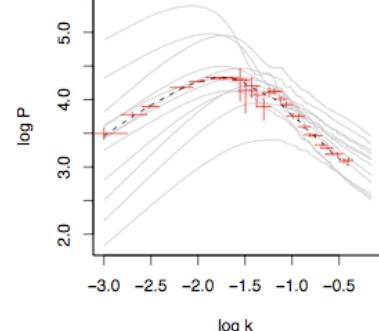
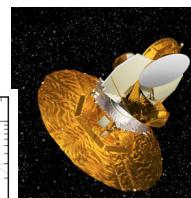
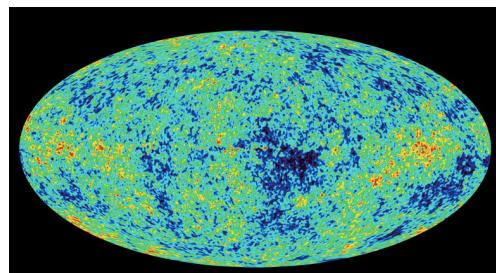


Combining observations and simulation models to inform about the cosmological model

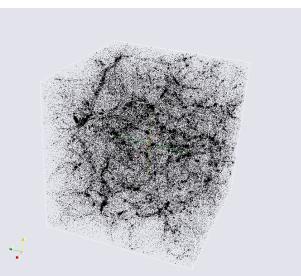
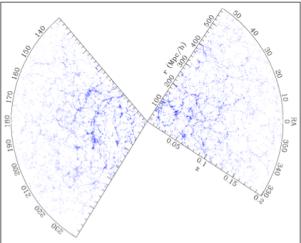
Sloan Digital Sky Survey



Wilkinson mass anisotropy probe

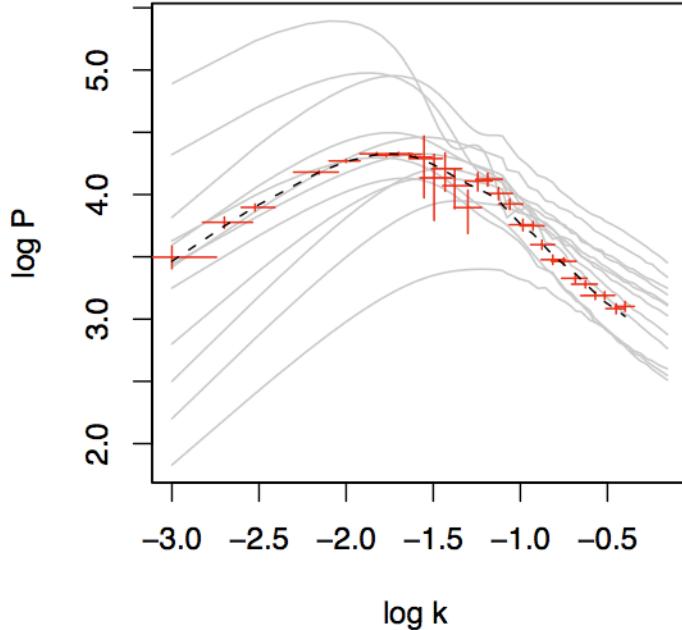


# Sloan Digital Sky Survey



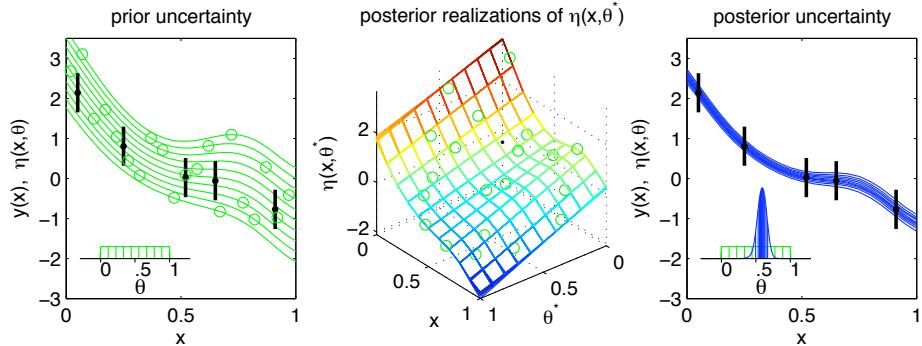
NATIONAL LABORATORY  
EST. 1943

data & simulated power spectra



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## Accounting for limited simulation runs

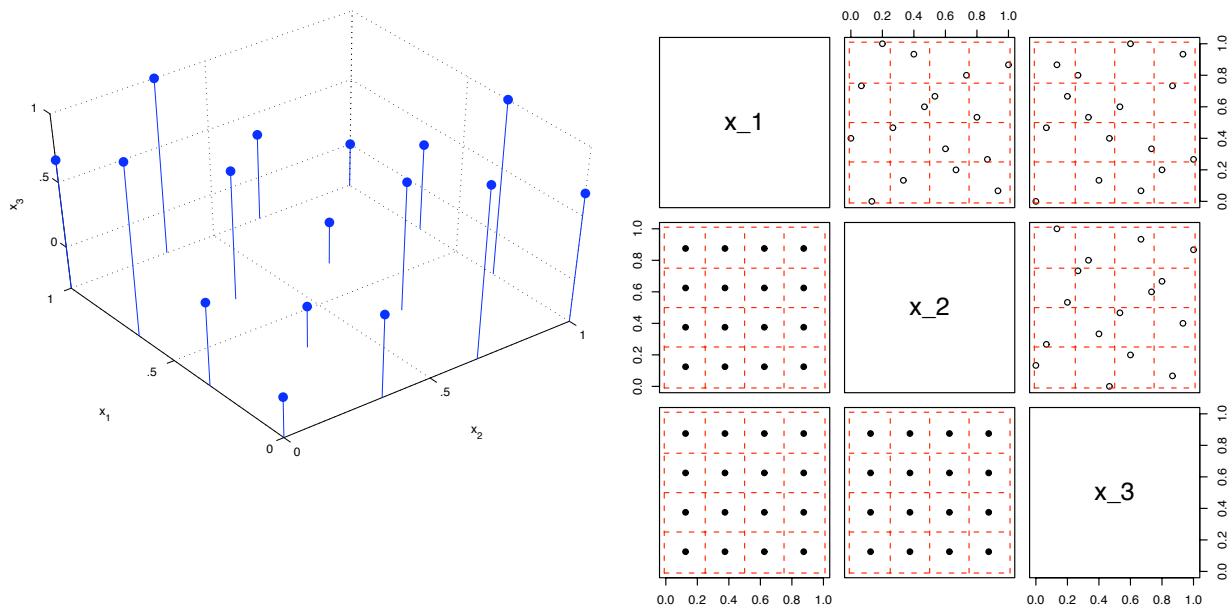


Again, standard Bayesian estimation gives:

$$\begin{aligned} \pi(\theta, \eta(\cdot, \cdot), \lambda_\epsilon, \rho_\eta, \lambda_\eta | y(x)) \propto & L(y(x) | \eta(x, \theta), \lambda_\epsilon) \times \\ & \pi(\theta) \times \pi(\eta(\cdot, \cdot) | \lambda_\eta, \rho_\eta) \\ & \pi(\lambda_\epsilon) \times \pi(\rho_\eta) \times \pi(\lambda_\eta) \end{aligned}$$

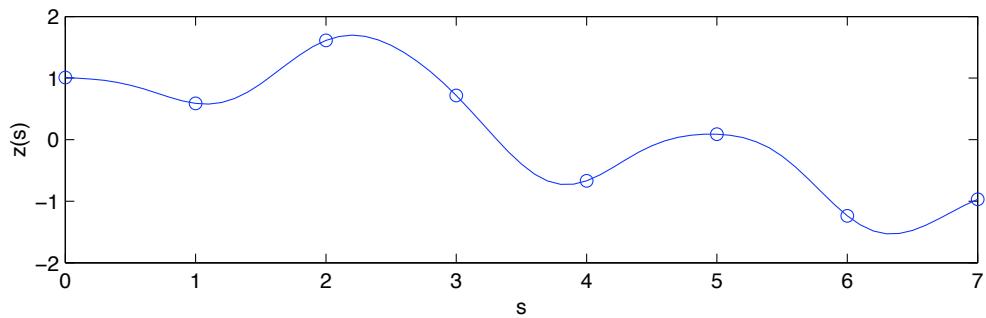
- Posterior means and quantiles shown.
- Uncertainty in  $\theta$ ,  $\eta(\cdot, \cdot)$ , nuisance parameters are incorporated into the forecast.
- Gaussian process models for  $\eta(\cdot, \cdot)$ .

# OA-based Latin Hypercube designs



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## Gaussian process models for spatial phenomena



An example of  $z(s)$  of a Gaussian process model on  $s_1, \dots, s_n$

$$z = \begin{pmatrix} z(s_1) \\ \vdots \\ z(s_n) \end{pmatrix} \sim N \left( \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma & & \\ & \ddots & \\ & & \Sigma \end{pmatrix} \right), \text{ with } \Sigma_{ij} = \exp\{-||s_i - s_j||^2\},$$

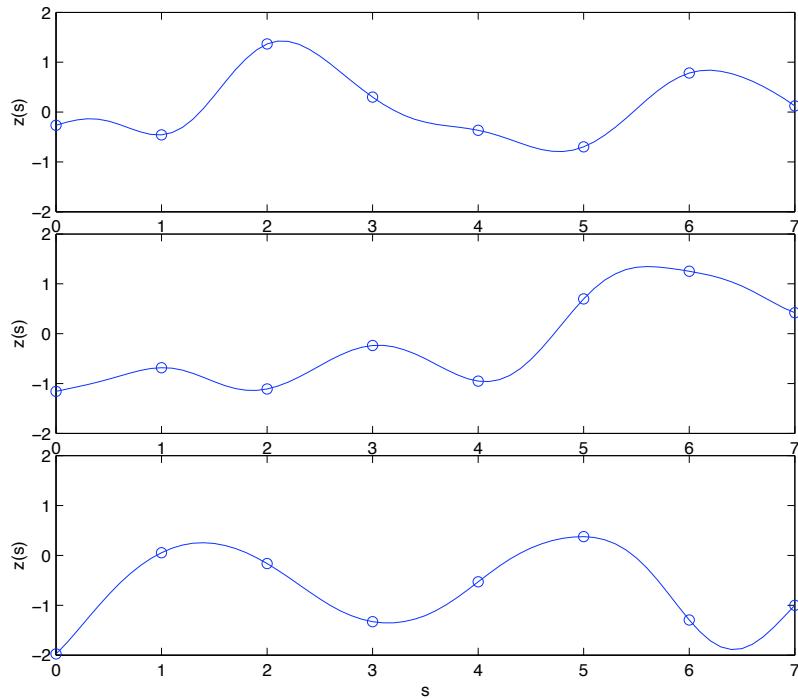
where  $||s_i - s_j||$  denotes the distance between locations  $s_i$  and  $s_j$ .

$z$  has density  $\pi(z) = (2\pi)^{-\frac{n}{2}} |\Sigma|^{-\frac{1}{2}} \exp\{-\frac{1}{2} z^T \Sigma^{-1} z\}$ .



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Realizations from  $\pi(z) = (2\pi)^{-\frac{n}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2} z^T \Sigma^{-1} z\right\}$



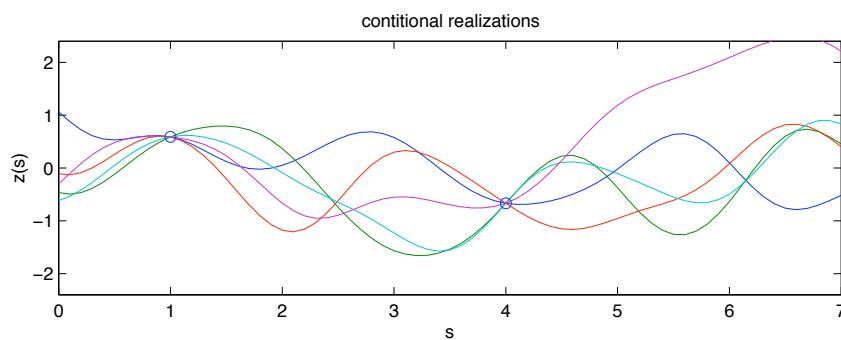
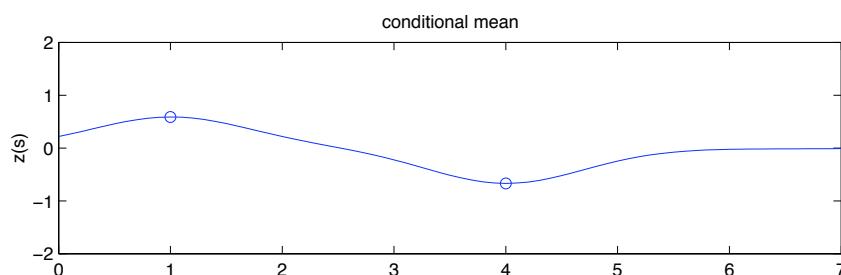
model for  $z(s)$  can be extended to continuous  $s$



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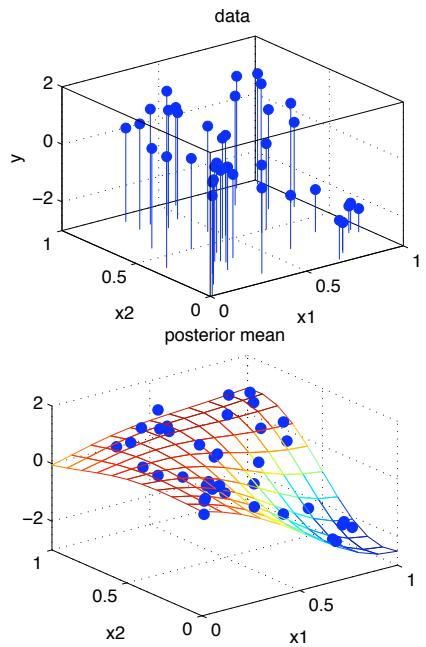
Conditioning on some observations of  $z(s)$

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \sim N \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right), \quad z_2 | z_1 \sim N(\Sigma_{21} \Sigma_{11}^{-1} z_1, \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12})$$

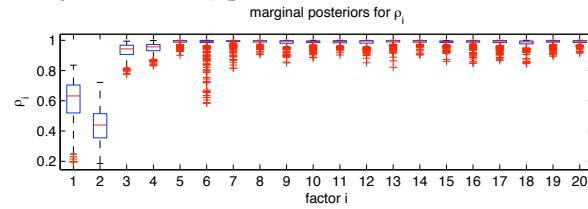


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## Emulating computer output using a Gaussian process



example:  $n = 40; p = 20$



Posterior for 1-d formulation:

$$\pi(\lambda_y, \lambda_\eta, \rho | y) \propto |\lambda_y^{-1} I_m + \lambda_w^{-1} R|^{-\frac{1}{2}} \exp\{-\frac{1}{2} y^T (\lambda_\eta^{-1} I_m + \lambda_w^{-1} R)^{-1} y\} \times \lambda_y^{ay-1} e^{-b_y \lambda_y} \times \lambda_\eta^{a_\eta-1} e^{-b_\eta \lambda_\eta} \times \prod_{j=1}^p (1 - \rho_j)^{b_\rho-1}$$

$$R((x, \theta), (x', \theta'); \rho) = \prod_{k=1}^{px} \rho_k^{4(x_k - x'_k)^2} \times \prod_{k=1}^{p\theta} \rho_{k+px}^{4(\theta_k - \theta'_k)^2}$$

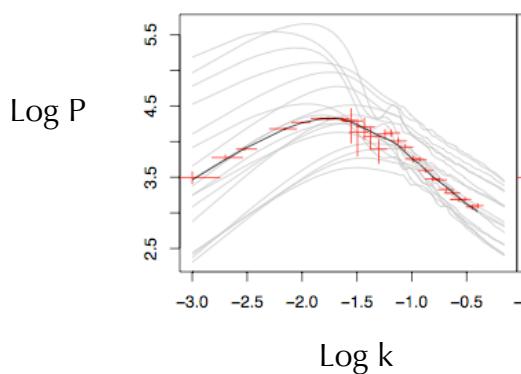
interpolating a smooth surface  $\Rightarrow p$  can be relatively large.

rule of thumb:  $n = 10 \times \#$  of active factors (Sacks, Welch, Mitchell, Wynn, 1989).

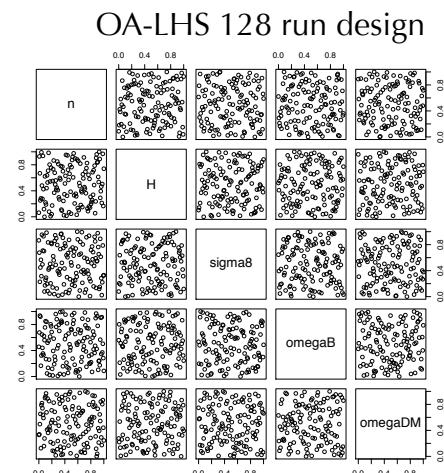


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## Data, parameter ranges, simulations



Synthetic data were generated from a “true” cosmology using both linear perturbation theory and the particle mesh code MC<sup>2</sup>



### Calibration parameter ranges

Spectral index	0.8 to 1.4
Hubble parameter	0.5 to 1.1
Sigma 8	0.6 to 1.6
Omega CDM	0.051 to 0.6
Omega baryon	0.02 to 0.12



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# Model of the data

$$y(k) = \eta(\theta; k) + \epsilon(k)$$

Posterior density:

$$\pi(\eta(\cdot; k), \theta, \xi | y) \propto L(y | \eta(\cdot, k), \theta, \Sigma_\epsilon) \times \pi(\eta(\cdot; k) | \xi) \times \pi(\theta) \times \pi(\xi)$$

$\Sigma_e$  is known,  $\xi$  controls statistical parameters governing  $\eta(\cdot; k)$ .

Posterior for cosmological parameters computed via MCMC

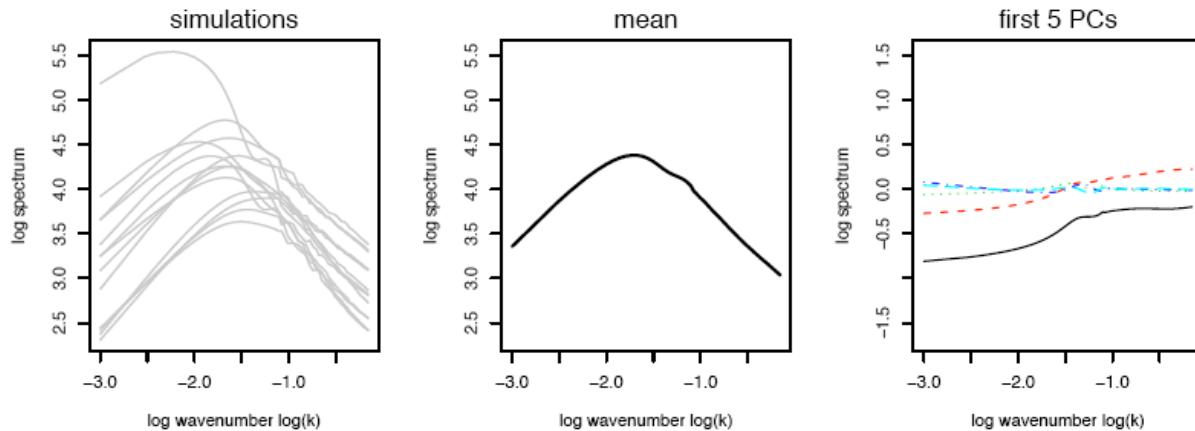
$$\pi(\theta | y) \propto \int \pi(\eta(\cdot; k), \theta, \xi | y) d\eta d\xi$$



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## Basis representation of simulated spectra

The power spectra resulting from the 128 simulations are used to construct a mean-adjusted principal component representation.



Power spectra are represented as a function of the 5-d input parameters  $\theta$  and PC basis functions  $\phi_j(k)$ :

$$\hat{\eta}(\theta; k) = \sum_{j=1}^{p_\eta} w_j(\theta) \phi_j(k)$$

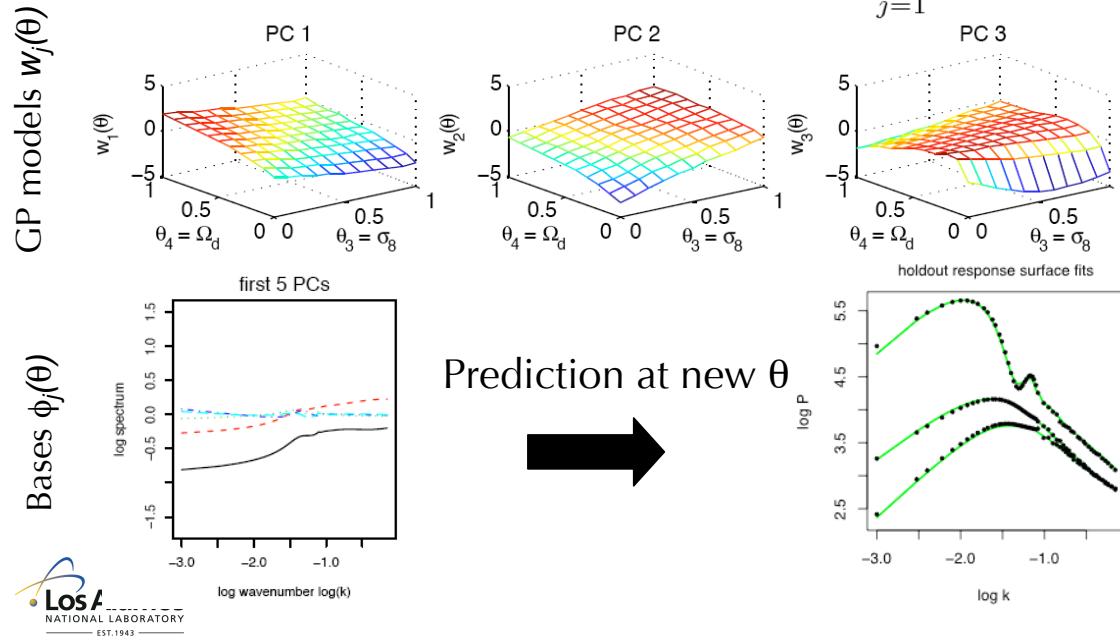


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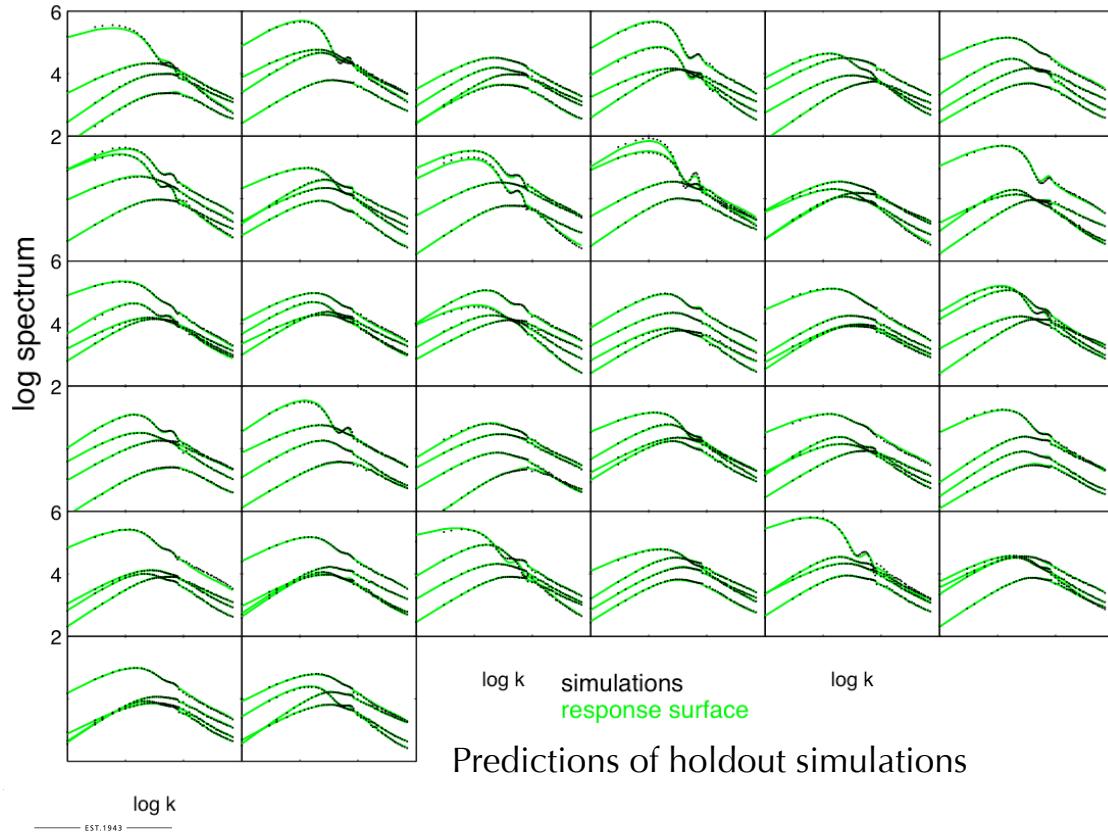
# Gaussian process model to emulate simulation output

Gaussian process (GP) models are used to estimate the weights  $w_j(\theta)$  at untried settings

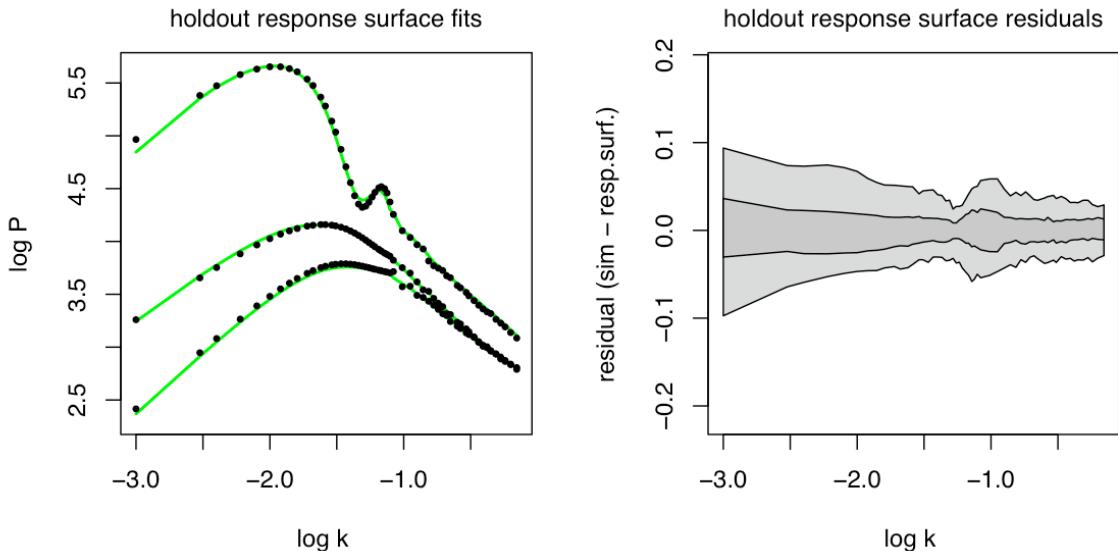
$$\hat{\eta}(\theta; k) = \sum_{j=1}^{p_\eta} w_j(\theta) \phi_j(k)$$



## Response surface accuracy

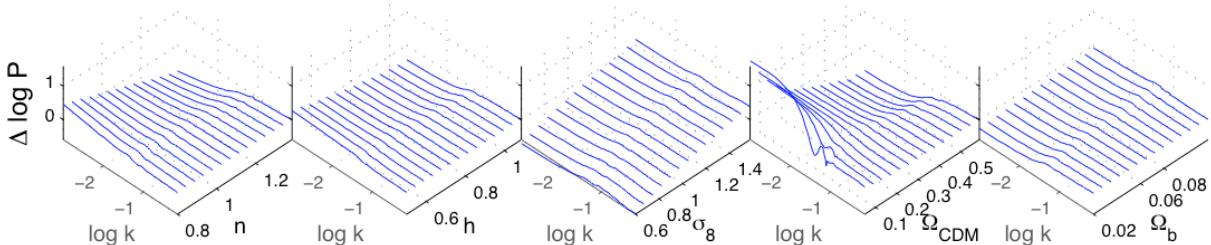


# Response surface accuracy



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## Simulator emulation and sensitivity



Changes in the emulator prediction as each parameter is varied while holding the others at their midpoint.

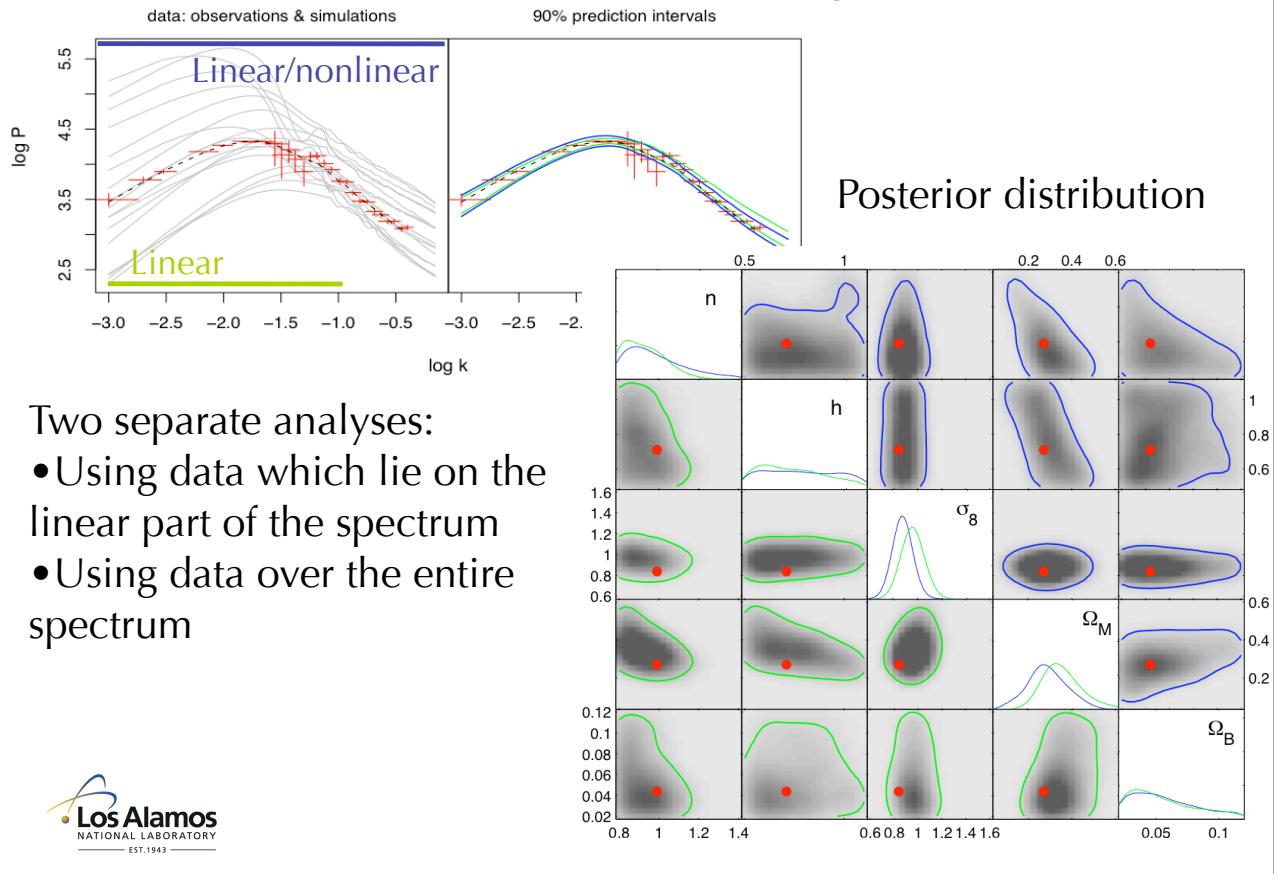
Note:  $\sigma_8$  and  $\Omega_{\text{CDM}}$  have the largest effect on  $\log P$

Only  $\sigma_8$  has a substantial effect on nonlinear part of the mass power spectrum ( $\log k < -1$ )



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# Calibration results for test problem



## Formulation (single experiment type)

calibration parameter vector

$$\theta \quad \pi(\theta)$$

statistical model parameters

$$\lambda \quad \pi(\lambda)$$

experimental data and simulation output

$$y \quad L(y|\theta, \lambda)$$

⇒ Posterior distribution

$$\pi(\theta, \lambda|y) \propto L(y|\theta, \lambda) \times \pi(\theta) \times \pi(\lambda)$$

Integrating over the statistical model parameters gives the marginal posterior for the calibration parameters  $\theta$ .

$$\pi(\theta|y) \propto \int L(y|\theta, \lambda) \times \pi(\theta) \times \pi(\lambda) d\lambda$$

Uncertainty in the parameters  $(\theta, \lambda)$  gives uncertainty in simulation-based predictions.

Prediction uncertainty also depends on how well simulations match reality.

## Formulation for combining different experiment types

Experiments have physical parameters  $\theta^*$  in common.

	expt 1	expt 2	model term
calibration parameter vector	$(\theta_1, \theta^*)$	$(\theta_2, \theta^*)$	$\pi(\theta_1, \theta_2, \theta^*)$
statistical model parameters		$\lambda_1$	$\lambda_2$
experimental data and simulation output		$y_1$	$y_2$

⇒ Posterior distribution

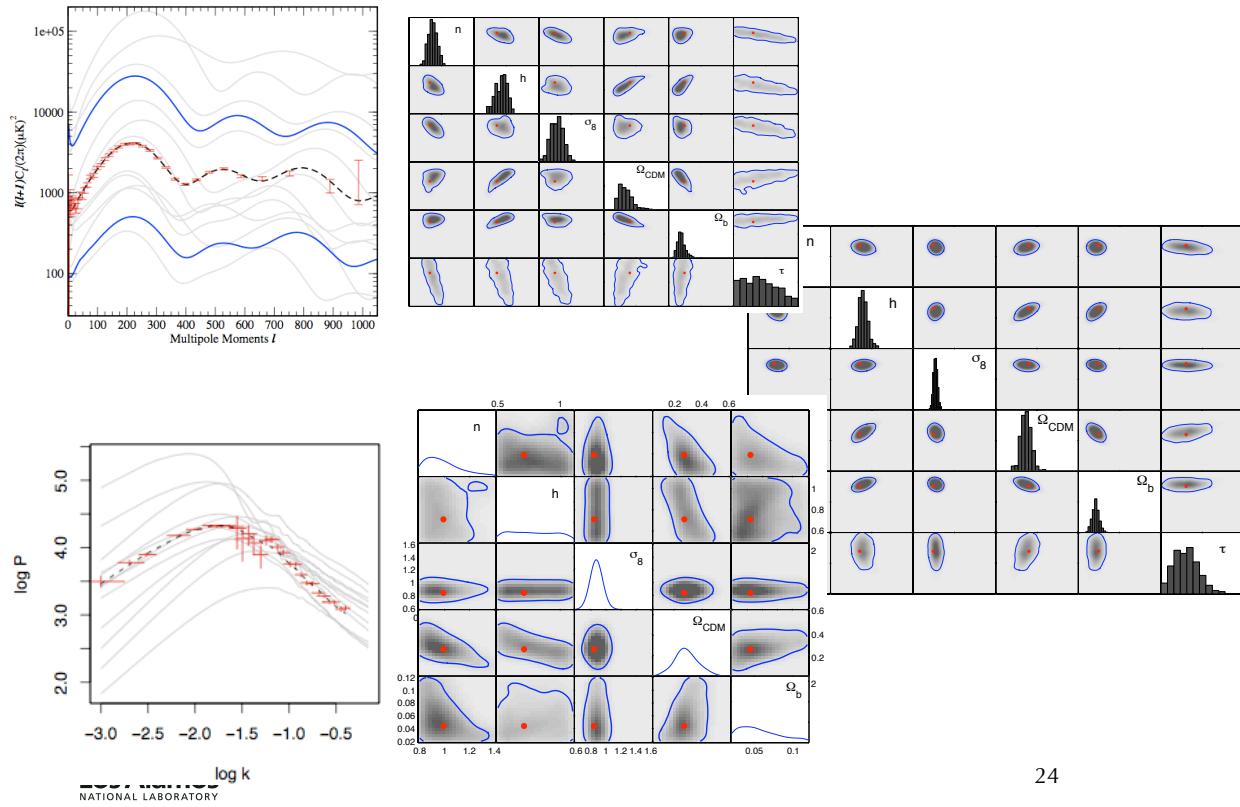
$$\begin{aligned} \pi(\theta, \lambda | y) &\propto L(y_1 | \theta_1, \theta^*, \lambda_1) \times L(y_2 | \theta_2, \theta^*, \lambda_2) \\ &\times \pi(\theta_1, \theta_2, \theta^*) \times \pi(\lambda_1) \times \pi(\lambda_2) \end{aligned}$$

- Both experiment types inform about common parameters  $\theta^*$ .
- Easily generalizes to multiple experiment types.
- May assign weights  $w_i \leq 1$  to likelihood terms  $L(y_i | \theta_i, \theta^*, \lambda_i)^{w_i}$  to control experiment's influence on calibration.



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## Combined WMAP & SDSS analysis



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# Ending points

- will look at other data sources & sim models (Lyman alpha forest, weak lensing)
- model inadequacy and data issues
- Compartmentalization
- Extrapolation

